Framework For Comparing Error Covariance Estimation Schemes

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Mathematical Approaches of Atmospheric Constituents Data Assimilation and Inverse Modeling workshop

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(Richard Ménard, ECCC)

Environnement Canada Environment Canada

Canada

Introduction

- Specification of error covariances can impact the quality of the analyses
  - Background error covariances $\mathbf{B}$
  - Observation error covariances $\mathbf{R}$

- Difficult to accurately specifying error covariances $\widetilde{\mathbf{B}}$ and $\widetilde{\mathbf{R}}$
  - Helpful to have methods to diagnose and/or tune the error covariances

- For simplicity, we focus on tuning variances only

$$\widetilde{\mathbf{B}}' = s_\mathrm{b}\widetilde{\mathbf{B}} \qquad \widetilde{\mathbf{R}}' = s_\mathrm{o}\widetilde{\mathbf{R}}$$

Observation-Space Residuals

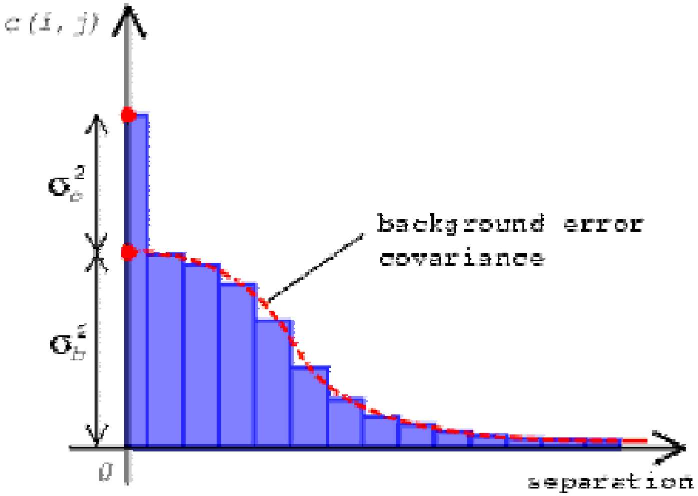
- The innovation vector $\mathbf{d}$ does not depend on the true variables

$$\mathbf{d} = \underset{\substack{\uparrow \\ \text{observations}}}{\mathbf{y}} - H(\underset{\substack{\uparrow \\ \text{background}}}{\mathbf{x}_\mathrm{b}}) \approx \boldsymbol{\epsilon}_\mathrm{o} - \underset{\substack{\uparrow \\ \text{linear obs.} \\ \text{operator}}}{\mathbf{H}}\boldsymbol{\epsilon}_\mathrm{b} \qquad \mathbf{D} = \mathrm{cov}(\mathbf{d}, \mathbf{d}) = \mathbf{HBH}^\mathrm{T} + \mathbf{R}$$

- However, $\mathbf{B}$ and $\mathbf{R}$ are not separate in $\mathbf{D}$
  - Want modelled quantities $\widetilde{\mathbf{B}}$ and $\widetilde{\mathbf{R}}$

Hollingsworth and Lönnberg

- Assumes we can attribute all spatial correlations in the innovation to the background
  - $\tilde{\mathbf{R}}$ assumes diagonal
  - $\tilde{\mathbf{B}}$ terms are fit to the observed innovation at nonzero spatial separation
  - Extrapolation to zero spatial separation



Bouttier, F., and P. Courtier. "Data assimilation concepts and methods March 1999." *Meteorological training course lecture series. ECMWF* 718 (2002): 59.

The Desroziers and Ivanov 2001 Method (DI01)

innovation covariance consistency $\mathrm{E}[\mathbf{D}] = \widetilde{\mathbf{D}}$

- For variational assimilation systems

$$\mathrm{E}[J_\mathrm{b}(\mathbf{x}_\mathrm{a})] = \tfrac{1}{2}\mathrm{Tr}[\mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^\mathrm{T}\widetilde{\mathbf{D}}^{-1}\mathrm{E}[\mathbf{D}]\widetilde{\mathbf{D}}^{-1}] \xrightarrow{\mathrm{E}[\mathbf{D}]=\widetilde{\mathbf{D}}} \tfrac{1}{2}\mathrm{Tr}[\mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^\mathrm{T}\widetilde{\mathbf{D}}^{-1}]$$

$$\mathrm{E}[J_\mathrm{o}(\mathbf{x}_\mathrm{a})] = \tfrac{1}{2}\mathrm{Tr}[\widetilde{\mathbf{R}}\widetilde{\mathbf{D}}^{-1}\mathrm{E}[\mathbf{D}]\widetilde{\mathbf{D}}^{-1}] \xrightarrow{\mathrm{E}[\mathbf{D}]=\widetilde{\mathbf{D}}} \tfrac{1}{2}\mathrm{Tr}[\widetilde{\mathbf{R}}\widetilde{\mathbf{D}}^{-1}]$$

- Iterative scheme:

$$(s_\mathrm{b}^\mathrm{DI01})_{i+1} = \frac{\mathrm{Tr}[\mathbf{H}\widetilde{\mathbf{B}}_i\mathbf{H}^\mathrm{T}\widetilde{\mathbf{D}}_i^{-1}\mathbf{D}\widetilde{\mathbf{D}}_i^{-1}]}{\mathrm{Tr}[\mathbf{H}\widetilde{\mathbf{B}}_i\mathbf{H}^\mathrm{T}\widetilde{\mathbf{D}}_i^{-1}]} \qquad (s_\mathrm{o}^\mathrm{DI01})_{i+1} = \frac{\mathrm{Tr}[\widetilde{\mathbf{R}}_i\widetilde{\mathbf{D}}_i^{-1}\mathbf{D}\widetilde{\mathbf{D}}_i^{-1}]}{\mathrm{Tr}[\widetilde{\mathbf{R}}_i\widetilde{\mathbf{D}}_i^{-1}]}$$

- Has been used in a NWP assimilation system, but difficult to implement due to high computational cost

The Desroziers et al. 2005 Method (D05)

$$\mathrm{E}[(\mathrm{H}(\mathbf{x}_\mathrm{a}) - \mathrm{H}(\mathbf{x}_\mathrm{b}))\mathbf{d}^\mathrm{T}] = \mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^\mathrm{T}\widetilde{\mathbf{D}}^{-1}\mathrm{E}[\mathbf{D}] \xrightarrow{\mathrm{E}[\mathbf{D}]=\widetilde{\mathbf{D}}} \mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^\mathrm{T}$$

$$\mathrm{E}[(\mathbf{y} - \mathrm{H}(\mathbf{x}_\mathrm{a}))\mathbf{d}^\mathrm{T}] = \widetilde{\mathbf{R}}\widetilde{\mathbf{D}}^{-1}\mathrm{E}[\mathbf{D}] \xrightarrow{\mathrm{E}[\mathbf{D}]=\widetilde{\mathbf{D}}} \widetilde{\mathbf{R}}$$

- Iterative scheme:

$$(s_\mathrm{b}^\mathrm{D05})_{i+1} = \frac{\mathrm{Tr}[\mathbf{H}\widetilde{\mathbf{B}}_i\mathbf{H}^\mathrm{T}\widetilde{\mathbf{D}}_i^{-1}\mathbf{D}]}{\mathrm{Tr}[\mathbf{H}\widetilde{\mathbf{B}}_i\mathbf{H}^\mathrm{T}]} \qquad (s_\mathrm{o}^\mathrm{D05})_{i+1} = \frac{\mathrm{Tr}[\widetilde{\mathbf{R}}_i\widetilde{\mathbf{D}}_i^{-1}\mathbf{D}]}{\mathrm{Tr}[\widetilde{\mathbf{R}}_i]}$$

- Typically much less computationally demanding than DI01

Method Comparisons

- Different methods can produce very different results
- For DI01 and D05, not evident exactly how **B** and **R** are being separated
- Mathematical formalism needed for:
  - Direct comparison between methods
    - Why do they work?
  - Understanding different regimes for each method:
    - When do each method give reasonable results or fail?

Filtering and the Analysis

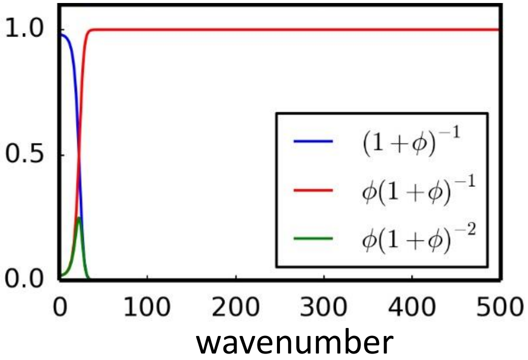
- Transform to basis that simultaneously diagonalizes and $\mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^{\mathrm{T}}$ and $\widetilde{\mathbf{R}}$

$$\phi = \frac{\text{spectra of } \widetilde{\mathbf{R}}}{\text{spectra of } \mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^{\mathrm{T}}}$$

- Construct operators:

$\tilde{\mathbf{F}}$ that dampens modes prominent in $\widetilde{\mathbf{R}}$ as compared to $\mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^{\mathrm{T}}$

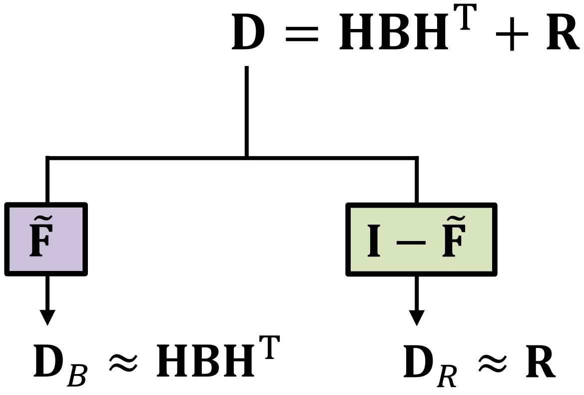
$\mathbf{I} - \tilde{\mathbf{F}}$ that dampens modes prominent in $\mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^{\mathrm{T}}$ as compared $\widetilde{\mathbf{R}}$



1D periodic domain of length $L = 40{,}000$ km, observations $\Delta x = 40$ km apart. $L_{\mathrm{b}} = 800$ km and $L_{\mathrm{o}} = 0$

$$\mathbf{H}\mathbf{x}_{\mathrm{a}} = \left(\mathbf{I} - \tilde{\mathbf{F}}\right)\mathbf{H}\mathbf{x}_{\mathrm{b}} + \tilde{\mathbf{F}}\mathbf{y} = \mathbf{H}\mathbf{x}_{\mathrm{b}} + \tilde{\mathbf{F}}\mathbf{d}$$

Filtering of Error Covariances



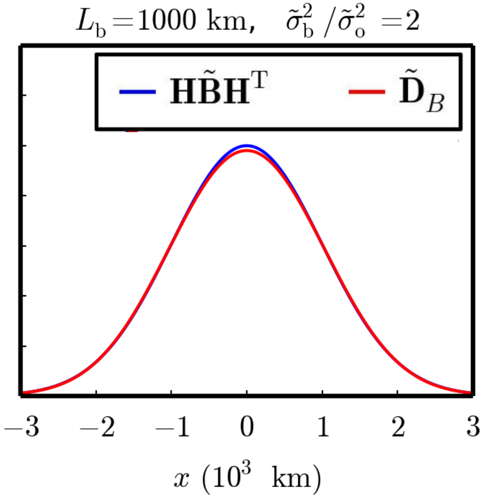
$$\mathbf{D} = \mathbf{HBH}^{\mathrm{T}} + \mathbf{R}$$

$\tilde{\mathbf{F}}$

$\mathbf{I} - \tilde{\mathbf{F}}$

$\mathbf{D}_B \approx \mathbf{HBH}^{\mathrm{T}}$

$\mathbf{D}_R \approx \mathbf{R}$



observed covariances

$$\mathbf{D}_B \equiv \tilde{\mathbf{F}}\mathbf{D}\tilde{\mathbf{F}}^{\mathrm{T}}$$

$$\mathbf{D}_R \equiv (\mathbf{I} - \tilde{\mathbf{F}})\mathbf{D}(\mathbf{I} - \tilde{\mathbf{F}})^{\mathrm{T}}$$

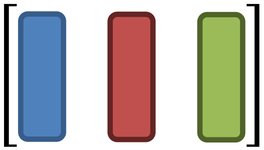
modelled covariances

$$\tilde{\mathbf{D}}_B \equiv \tilde{\mathbf{F}}\tilde{\mathbf{D}}\tilde{\mathbf{F}}^{\mathrm{T}}$$

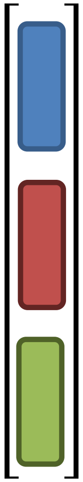
$$\tilde{\mathbf{D}}_R \equiv (\mathbf{I} - \tilde{\mathbf{F}})\tilde{\mathbf{D}}(\mathbf{I} - \tilde{\mathbf{F}})^{\mathrm{T}}$$

Vectorization of Matrices

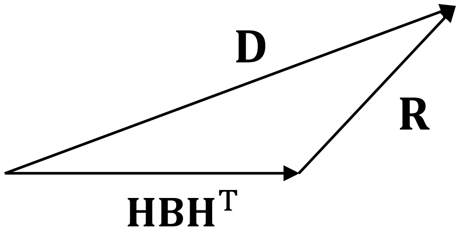
$\mathbf{A} =$



$\mathrm{vec}(\mathbf{A}) =$



$$\mathbf{D} = \mathbf{HBH}^{\mathrm{T}} + \mathbf{R}$$



Frobenius inner product: $\langle \mathbf{A}, \mathbf{B} \rangle = \mathrm{vec}(\mathbf{A}) \cdot \mathrm{vec}(\mathbf{B}) = \mathrm{Tr}[\mathbf{A}^{\mathrm{T}}\mathbf{B}]$

Linear Least-Squares Solution

$$\mathbf{y} = \mathbf{M}x + \boldsymbol{\epsilon}, \quad \mathrm{cov}(\boldsymbol{\epsilon}, \boldsymbol{\epsilon}) = \mathbf{C}$$

linear least-squares solution is $\hat{x} = \frac{\mathbf{M}^{\mathrm{T}}\mathbf{C}^{-1}\mathbf{y}}{\mathbf{M}^{\mathrm{T}}\mathbf{C}^{-1}\mathbf{M}}$

$$s_{\mathrm{o}}^{\mathrm{DI01}} = \frac{\overbrace{\mathrm{vec}\left(\widetilde{\mathbf{D}}_R\right)}^{\text{model}}{}^{\mathrm{T}}\,\overbrace{(\widetilde{\mathbf{D}}_R \otimes \widetilde{\mathbf{R}})}^{\text{covariance}}{}^{-1}\,\overbrace{\mathrm{vec}(\mathbf{D}_R)}^{\text{observed data}}}{\mathrm{vec}\left(\widetilde{\mathbf{D}}_R\right)^{\mathrm{T}}(\widetilde{\mathbf{D}}_R \otimes \widetilde{\mathbf{R}})^{-1}\mathrm{vec}(\widetilde{\mathbf{D}}_R)}$$

Linear Least-Squares Solution

$$\boxed{J_\mathrm{o} = \frac{1}{2}\|\mathbf{d}-\mathbf{H}\Delta\mathbf{x}\,\|^2_{\tilde{\mathbf{R}}^{-1}}}$$

$$J_R^{\mathrm{DI01}} \equiv \frac{1}{2}\left\|s_\mathrm{o}\tilde{\mathbf{D}}_R-\mathbf{D}_R\right\|^2_{(\tilde{\mathbf{D}}_R\otimes\tilde{\mathbf{R}})^{-1}}$$

minimize
w.r.t.
s_o

$$s_\mathrm{o}^{\mathrm{DI01}} = \frac{\overbrace{\mathrm{vec}\left(\tilde{\mathbf{D}}_R\right)^\mathrm{T}}^{\text{model}}\overbrace{(\tilde{\mathbf{D}}_R\otimes\tilde{\mathbf{R}})^{-1}}^{\text{covariance}}\overbrace{\mathrm{vec}(\mathbf{D}_R)}^{\text{observed data}}}{\mathrm{vec}\left(\tilde{\mathbf{D}}_R\right)^\mathrm{T}(\tilde{\mathbf{D}}_R\otimes\tilde{\mathbf{R}})^{-1}\mathrm{vec}(\tilde{\mathbf{D}}_R)}$$

$$J_B^{\mathrm{DI01}} \equiv \frac{1}{2}\left\|s_\mathrm{b}\tilde{\mathbf{D}}_B - \mathbf{D}_B\right\|^2_{(\tilde{\mathbf{D}}_B \otimes (\mathbf{H}\tilde{\mathbf{B}}\mathbf{H}^\mathrm{T}))^{-1}}$$

minimize
w.r.t.
s_b

$$s_\mathrm{b}^{\mathrm{DI01}} = \frac{\mathrm{vec}\left(\tilde{\mathbf{D}}_B\right)^\mathrm{T}(\tilde{\mathbf{D}}_B \otimes (\mathbf{H}\tilde{\mathbf{B}}\mathbf{H}^\mathrm{T}))^{-1}\mathrm{vec}(\mathbf{D}_B)}{\mathrm{vec}\left(\tilde{\mathbf{D}}_B\right)^\mathrm{T}(\tilde{\mathbf{D}}_B \otimes (\mathbf{H}\tilde{\mathbf{B}}\mathbf{H}^\mathrm{T}))^{-1}\mathrm{vec}(\tilde{\mathbf{D}}_B)}$$

$$J_R^{\mathrm{DI01}} \equiv \frac{1}{2}\left\|s_\mathrm{o}\tilde{\mathbf{D}}_R - \mathbf{D}_R\right\|^2_{(\tilde{\mathbf{D}}_R \otimes \tilde{\mathbf{R}})^{-1}}$$

minimize
w.r.t.
s_o

$$s_\mathrm{o}^{\mathrm{DI01}} = \frac{\mathrm{vec}\left(\tilde{\mathbf{D}}_R\right)^\mathrm{T}(\tilde{\mathbf{D}}_R \otimes \tilde{\mathbf{R}})^{-1}\mathrm{vec}(\mathbf{D}_R)}{\mathrm{vec}\left(\tilde{\mathbf{D}}_R\right)^\mathrm{T}(\tilde{\mathbf{D}}_R \otimes \tilde{\mathbf{R}})^{-1}\mathrm{vec}(\tilde{\mathbf{D}}_R)}$$

$$J_B^{\mathrm{D05}} \equiv \frac{1}{2}\left\|s_\mathrm{b}\tilde{\mathbf{D}}_B - \mathbf{D}_B\right\|^2_{(\tilde{\mathbf{B}}_B \otimes \mathbf{I})^{-1}}$$

minimize
w.r.t.
s_b

$$s_\mathrm{b}^{\mathrm{D05}} = \frac{\mathrm{vec}\left(\tilde{\mathbf{D}}_B\right)^\mathrm{T}(\tilde{\mathbf{B}}_B \otimes \mathbf{I})^{-1}\mathrm{vec}(\mathbf{D}_B)}{\mathrm{vec}\left(\tilde{\mathbf{D}}_B\right)^\mathrm{T}(\tilde{\mathbf{B}}_B \otimes \mathbf{I})^{-1}\mathrm{vec}(\tilde{\mathbf{D}}_B)}$$

$$J_R^{\mathrm{D05}} \equiv \frac{1}{2}\left\|s_\mathrm{o}\tilde{\mathbf{D}}_R - \mathbf{D}_R\right\|^2_{(\tilde{\mathbf{R}}_R \otimes \mathbf{I})^{-1}}$$

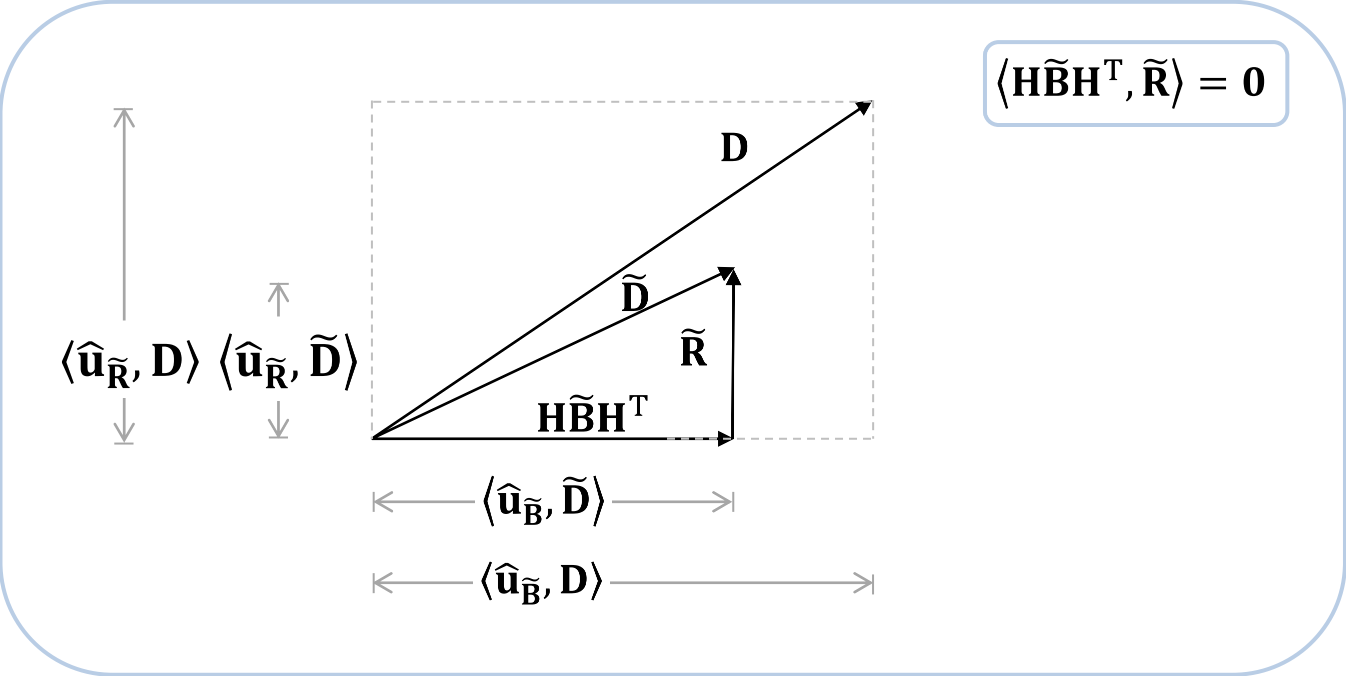
minimize
w.r.t.
s_o

$$s_\mathrm{o}^{\mathrm{D05}} = \frac{\mathrm{vec}\left(\tilde{\mathbf{D}}_R\right)^\mathrm{T}(\tilde{\mathbf{R}}_R \otimes \mathbf{I})^{-1}\mathrm{vec}(\mathbf{D}_R)}{\mathrm{vec}\left(\tilde{\mathbf{D}}_R\right)^\mathrm{T}(\tilde{\mathbf{R}}_R \otimes \mathbf{I})^{-1}\mathrm{vec}(\tilde{\mathbf{D}}_R)}$$

Geometric Interpretations

$$s_{\mathrm{b}}^{\mathrm{DI01}} = \frac{\langle \hat{\mathbf{u}}_{\tilde{\mathbf{B}}}, \mathbf{D} \rangle_{(\tilde{\mathbf{D}} \otimes \tilde{\mathbf{D}})^{-1}}}{\langle \hat{\mathbf{u}}_{\tilde{\mathbf{B}}}, \tilde{\mathbf{D}} \rangle_{(\tilde{\mathbf{D}} \otimes \tilde{\mathbf{D}})^{-1}}} \qquad s_{\mathrm{o}}^{\mathrm{DI01}} = \frac{\langle \hat{\mathbf{u}}_{\tilde{\mathbf{R}}}, \mathbf{D} \rangle_{(\tilde{\mathbf{D}} \otimes \tilde{\mathbf{D}})^{-1}}}{\langle \hat{\mathbf{u}}_{\tilde{\mathbf{R}}}, \tilde{\mathbf{D}} \rangle_{(\tilde{\mathbf{D}} \otimes \tilde{\mathbf{D}})^{-1}}}$$

$$s_{\mathrm{b}}^{\mathrm{D05}} = \frac{\langle \hat{\mathbf{u}}_{\tilde{\mathbf{B}}}, \mathbf{D} \rangle_{(\tilde{\mathbf{D}} \otimes \mathbf{I})^{-1}}}{\langle \hat{\mathbf{u}}_{\tilde{\mathbf{B}}}, \tilde{\mathbf{D}} \rangle_{(\tilde{\mathbf{D}} \otimes \mathbf{I})^{-1}}} \qquad s_{\mathrm{o}}^{\mathrm{D05}} = \frac{\langle \hat{\mathbf{u}}_{\tilde{\mathbf{R}}}, \mathbf{D} \rangle_{(\tilde{\mathbf{D}} \otimes \mathbf{I})^{-1}}}{\langle \hat{\mathbf{u}}_{\tilde{\mathbf{R}}}, \tilde{\mathbf{D}} \rangle_{(\tilde{\mathbf{D}} \otimes \mathbf{I})^{-1}}}$$

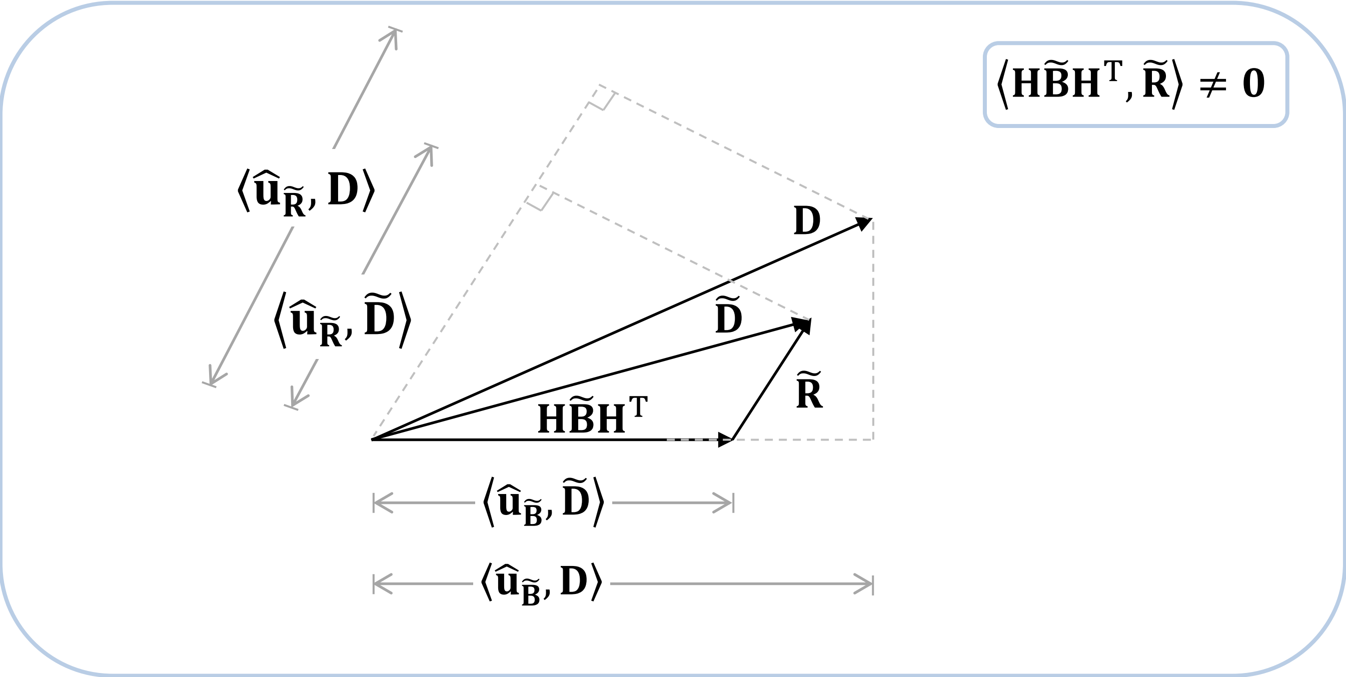


$$\boxed{\langle \mathbf{H}\tilde{\mathbf{B}}\mathbf{H}^{\mathrm{T}}, \tilde{\mathbf{R}} \rangle = \mathbf{0}}$$

Geometric Interpretations

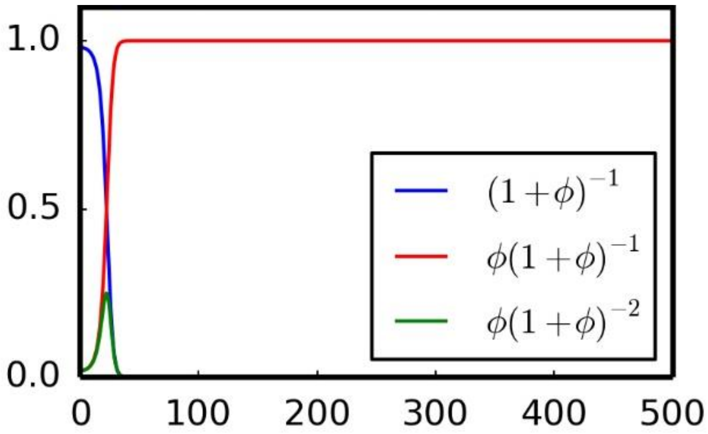
$$s_{\mathrm{b}}^{\mathrm{DI01}} = \frac{\langle \hat{\mathbf{u}}_{\widetilde{\mathbf{B}}}, \mathbf{D} \rangle_{(\widetilde{\mathbf{D}} \otimes \widetilde{\mathbf{D}})^{-1}}}{\langle \hat{\mathbf{u}}_{\widetilde{\mathbf{B}}}, \widetilde{\mathbf{D}} \rangle_{(\widetilde{\mathbf{D}} \otimes \widetilde{\mathbf{D}})^{-1}}} \qquad s_{\mathrm{o}}^{\mathrm{DI01}} = \frac{\langle \hat{\mathbf{u}}_{\widetilde{\mathbf{R}}}, \mathbf{D} \rangle_{(\widetilde{\mathbf{D}} \otimes \widetilde{\mathbf{D}})^{-1}}}{\langle \hat{\mathbf{u}}_{\widetilde{\mathbf{R}}}, \widetilde{\mathbf{D}} \rangle_{(\widetilde{\mathbf{D}} \otimes \widetilde{\mathbf{D}})^{-1}}}$$

$$s_{\mathrm{b}}^{\mathrm{D05}} = \frac{\langle \hat{\mathbf{u}}_{\widetilde{\mathbf{B}}}, \mathbf{D} \rangle_{(\widetilde{\mathbf{D}} \otimes \mathbf{I})^{-1}}}{\langle \hat{\mathbf{u}}_{\widetilde{\mathbf{B}}}, \widetilde{\mathbf{D}} \rangle_{(\widetilde{\mathbf{D}} \otimes \mathbf{I})^{-1}}} \qquad s_{\mathrm{o}}^{\mathrm{D05}} = \frac{\langle \hat{\mathbf{u}}_{\widetilde{\mathbf{R}}}, \mathbf{D} \rangle_{(\widetilde{\mathbf{D}} \otimes \mathbf{I})^{-1}}}{\langle \hat{\mathbf{u}}_{\widetilde{\mathbf{R}}}, \widetilde{\mathbf{D}} \rangle_{(\widetilde{\mathbf{D}} \otimes \mathbf{I})^{-1}}}$$

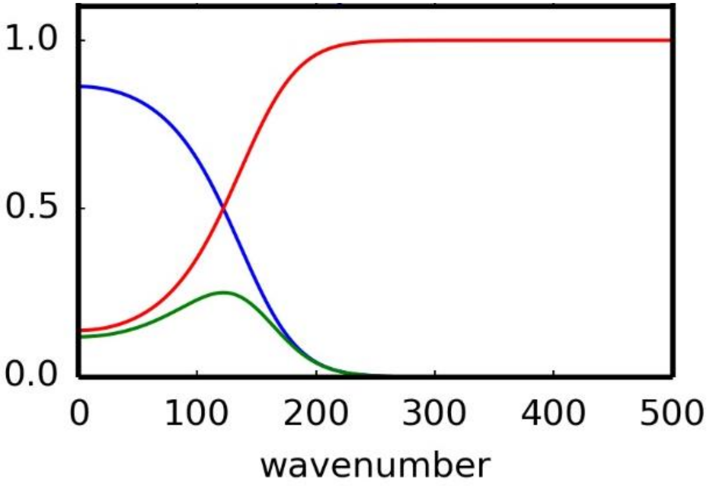


$$\boxed{\langle \mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^{\mathrm{T}}, \widetilde{\mathbf{R}} \rangle \neq \mathbf{0}}$$

Spectral Distinctiveness of Filters

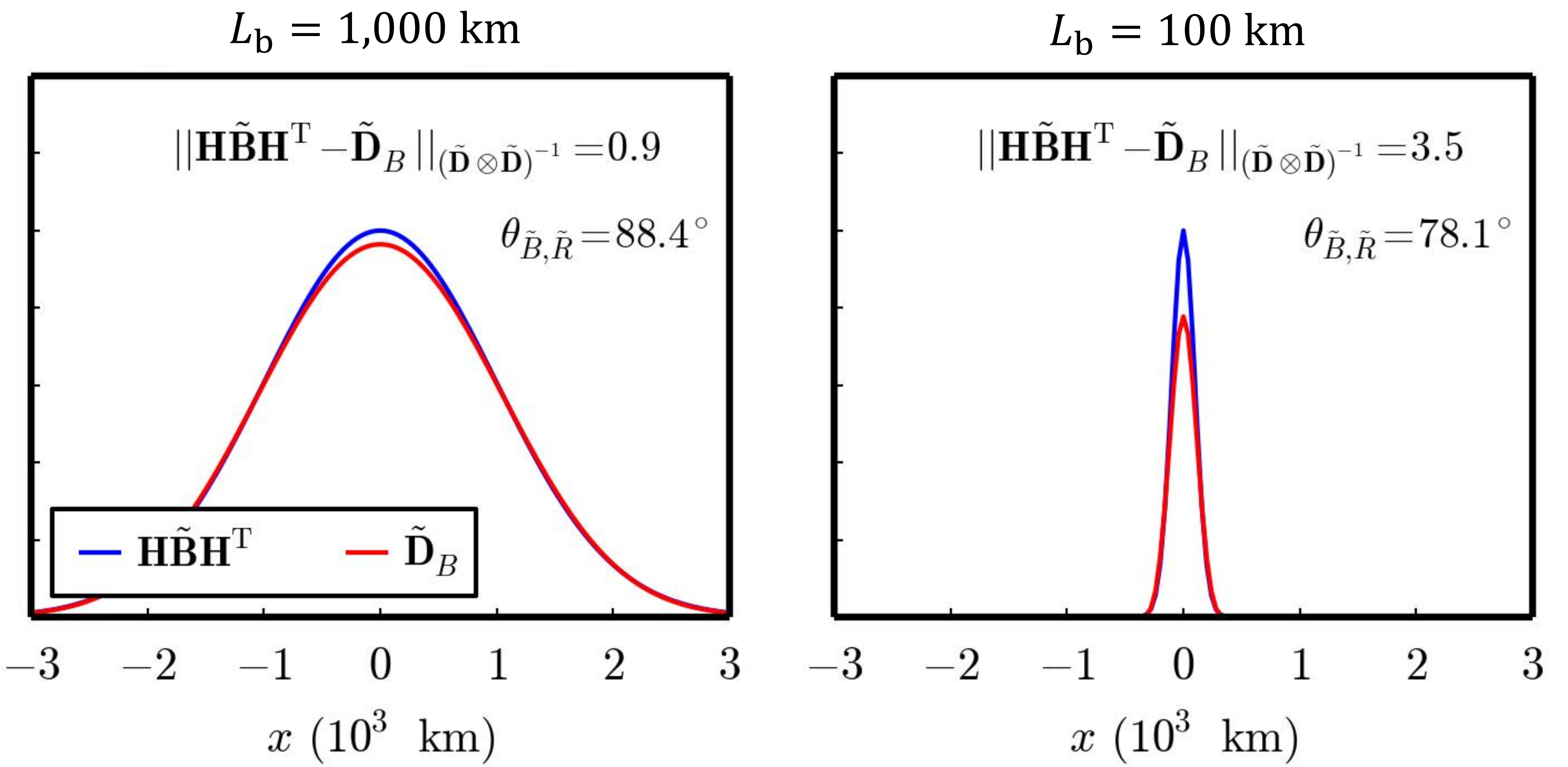

$L_\mathrm{b} = 800$ km

$$\theta_{\tilde{B},\tilde{R}} = 88°$$


$L_\mathrm{b} = 120$ km

$$\theta_{\tilde{B},\tilde{R}} = 78°$$

Error Covariance Filtering Efficiency



$L_\mathrm{b} = 1{,}000$ km

$L_\mathrm{b} = 100$ km

$L = 40{,}000$ km, $\tilde{\sigma}_\mathrm{b}^2 = \tilde{\sigma}_\mathrm{o}^2$, $L_\mathrm{o} = 0$

Statistical Properties

$$\frac{\mathrm{E}[s_{\mathrm{b}}^{\mathrm{DI01}}]}{s_{\mathrm{b}}^{\mathrm{t}}} = 1 + \left(\frac{s_{\mathrm{o}}^{\mathrm{t}}}{s_{\mathrm{b}}^{\mathrm{t}}} - 1\right) \frac{\left\langle \mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^{\mathrm{T}}, \widetilde{\mathbf{R}} \right\rangle_{(\widetilde{\mathbf{D}}\otimes\widetilde{\mathbf{D}})^{-1}}}{\left\langle \mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^{\mathrm{T}}, \widetilde{\mathbf{D}} \right\rangle_{(\widetilde{\mathbf{D}}\otimes\widetilde{\mathbf{D}})^{-1}}}$$

$$\frac{\mathrm{E}[s_{\mathrm{o}}^{\mathrm{DI01}}]}{s_{\mathrm{o}}^{\mathrm{t}}} = 1 + \left(\frac{s_{\mathrm{b}}^{\mathrm{t}}}{s_{\mathrm{o}}^{\mathrm{t}}} - 1\right) \frac{\left\langle \mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^{\mathrm{T}}, \widetilde{\mathbf{R}} \right\rangle_{(\widetilde{\mathbf{D}}\otimes\widetilde{\mathbf{D}})^{-1}}}{\left\langle \widetilde{\mathbf{R}}, \widetilde{\mathbf{D}} \right\rangle_{(\widetilde{\mathbf{D}}\otimes\widetilde{\mathbf{D}})^{-1}}}$$

$$\mathrm{V}\left[\frac{s_{\mathrm{b}}^{\mathrm{DI01}}}{s_{\mathrm{b}}^{\mathrm{t}}}\right] = \frac{2\mathrm{Tr}\left[\left(\mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^{\mathrm{T}}\widetilde{\mathbf{D}}^{-1}\left(\mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^{\mathrm{T}} + \frac{s_{\mathrm{o}}^{\mathrm{t}}}{s_{\mathrm{b}}^{\mathrm{t}}}\widetilde{\mathbf{R}}\right)\widetilde{\mathbf{D}}^{-1}\right)^{2}\right]}{\mathrm{Tr}\left[\mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^{\mathrm{T}}\widetilde{\mathbf{D}}^{-1}\right]^{2}}$$

$$\mathrm{V}\left[\frac{s_{\mathrm{o}}^{\mathrm{DI01}}}{s_{\mathrm{o}}^{\mathrm{t}}}\right] = \frac{2\mathrm{Tr}\left[\left(\widetilde{\mathbf{R}}\widetilde{\mathbf{D}}^{-1}\left(\frac{s_{\mathrm{b}}^{\mathrm{t}}}{s_{\mathrm{o}}^{\mathrm{t}}}\mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^{\mathrm{T}} + \widetilde{\mathbf{R}}\right)\widetilde{\mathbf{D}}^{-1}\right)^{2}\right]}{\mathrm{Tr}\left[\widetilde{\mathbf{R}}\widetilde{\mathbf{D}}^{-1}\right]^{2}}$$

*case where correlations are properly specified

Evaluating Expected Performance

- Case 1:
  - Model error covariances with $L_\mathrm{b} = 1{,}000\ \mathrm{km}$
  - Using observed innovations, calculated $s_\mathrm{b}^\mathrm{DI01} = 2.6$ and $s_\mathrm{o}^\mathrm{DI01} = 1.3$

$\theta_{\tilde{B},\tilde{R}} = 83^\circ$ ⇨

$\mathrm{RMSE}\left[s_\mathrm{b}^\mathrm{DI01}\right] \approx 17\%$

$\mathrm{RMSE}\left[s_\mathrm{o}^\mathrm{DI01}\right] \approx 4\%$

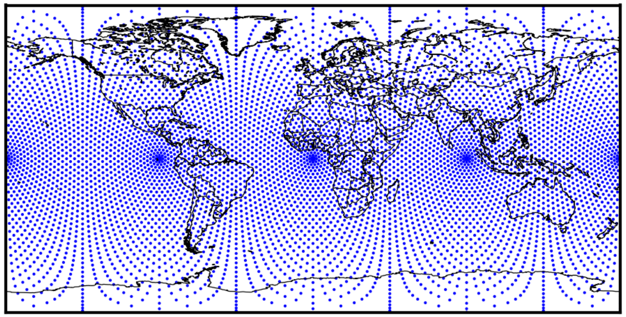
- Case 2:
  - Model error covariances with $L_\mathrm{b} = 250\ \mathrm{km}$
  - Using observed innovations, calculated $s_\mathrm{b}^\mathrm{DI01} = 3.3$ and $s_\mathrm{o}^\mathrm{DI01} = 1.1$

$\theta_{\tilde{B},\tilde{R}} = 26^\circ$ ⇨

$\mathrm{RMSE}\left[s_\mathrm{b}^\mathrm{DI01}\right] \approx 35\%$

$\mathrm{RMSE}\left[s_\mathrm{o}^\mathrm{DI01}\right] \approx 84\%$

Model error covariances $\tilde{\sigma}_\mathrm{b}^2 = \tilde{\sigma}_\mathrm{o}^2$ and $L_\mathrm{o} = 0$



5810-point Lebedev grid, $\Delta x \sim 100\ \mathrm{km} - 330\ \mathrm{km}$

Generalized Algorithm

- DI01 and D05 part of a larger class of algorithm, each defined by their choice of weights

$$\hat{s}_\mathrm{b} = \frac{\mathrm{vec}\left(\widetilde{\mathbf{D}}_B\right)^\mathrm{T}(\mathbf{W}_1 \otimes \mathbf{W}_2)\mathrm{vec}(\mathbf{D}_B)}{\mathrm{vec}\left(\widetilde{\mathbf{D}}_B\right)^\mathrm{T}(\mathbf{W}_1 \otimes \mathbf{W}_2)\mathrm{vec}(\widetilde{\mathbf{D}}_B)} \qquad \hat{s}_\mathrm{o} = \frac{\mathrm{vec}\left(\widetilde{\mathbf{D}}_R\right)^\mathrm{T}(\mathbf{W}_1 \otimes \mathbf{W}_2)\mathrm{vec}(\mathbf{D}_R)}{\mathrm{vec}\left(\widetilde{\mathbf{D}}_R\right)^\mathrm{T}(\mathbf{W}_1 \otimes \mathbf{W}_2)\mathrm{vec}(\widetilde{\mathbf{D}}_R)}$$

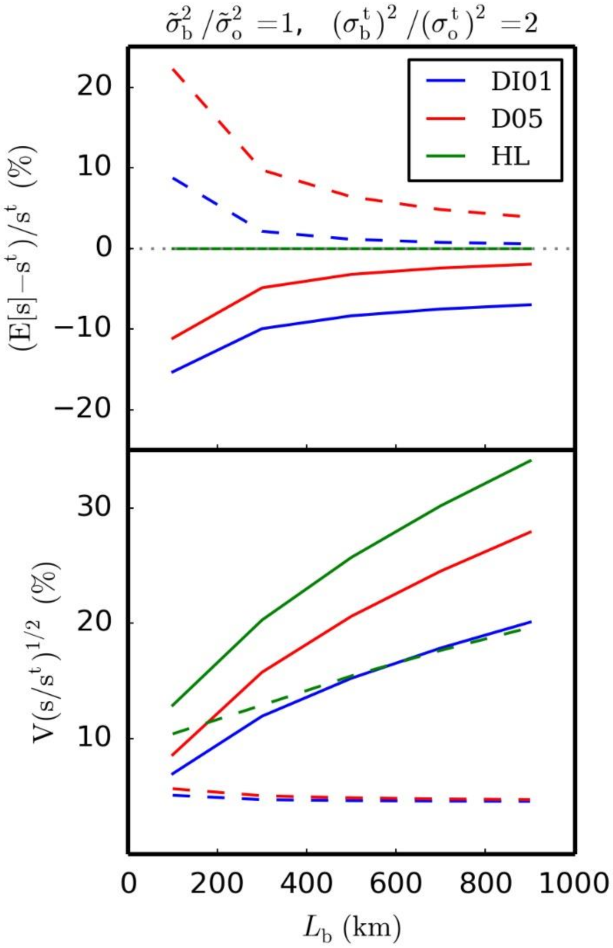
- Weighting of $(\widetilde{\mathbf{D}}_B \otimes \widetilde{\mathbf{D}}_B)^{-1}$ and $(\widetilde{\mathbf{D}}_R \otimes \widetilde{\mathbf{D}}_R)^{-1}$gives algorithm to satisfy the χ^2 diagnostic with $\hat{s}_\mathrm{b} = \hat{s}_\mathrm{o}$

Weighting in Least-Squares Fitting

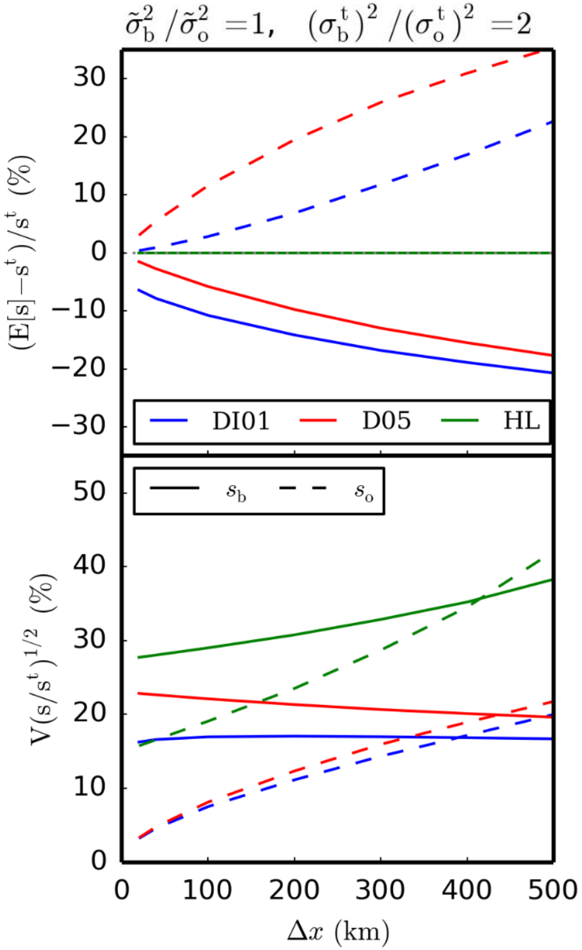
- If $\mathbf{d} \sim \mathcal{N}(\mathbf{0}, \mathbf{D})$, then the sample covariance $\boldsymbol{S}$ follows a Wishart distribution with $V[S_{i,j}] \propto D_{i,j}^2 + D_{i,i}D_{j,j}$

Method	J_B weighting	J_R weighting
DI01	$(\widetilde{\mathbf{D}}_B \otimes (\mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^{\mathrm{T}}))^{-1}$	$(\widetilde{\mathbf{D}}_R \otimes \widetilde{\mathbf{R}})^{-1}$
D05	$(\widetilde{\mathbf{B}}_B \otimes \mathbf{I})^{-1}$	$(\widetilde{\mathbf{R}}_R \otimes \mathbf{I})^{-1}$
χ^2	$(\widetilde{\mathbf{D}}_B \otimes \widetilde{\mathbf{D}}_B)^{-1}$	$(\widetilde{\mathbf{D}}_R \otimes \widetilde{\mathbf{D}}_R)^{-1}$

Comparisons Between Methods



1D periodic domain
$L = 40{,}000$ km, $\Delta x = 40$ km , $L_{\rm o} = 0$



1D periodic domain
$L = 40{,}000$ km, $L_{\rm b} = 600$ km , $L_{\rm o} = 0$

Conclusions

- DI01, D05, and HL all fit modelled to observation error covariances
  - Fitting is explicit for HL, implicit for DI01 and D05
- Conceptually, DI01 and D05 only differ by the weighting of the cost functions
  - Numerical differences between DI01 and D05 are important
- Performance of DI01 and D05 can be quantified through geometric quantities like $\theta_{\tilde{B},\tilde{R}}$
- Analytic results for error covariances scaling statistics

Sitwell, Michael, and Richard Ménard. "Framework for the comparison of a priori and a posteriori error variance estimation and tuning schemes." *Quarterly Journal of the Royal Meteorological Society* 146.731 (2020): 2547-2575.

Extra Slides

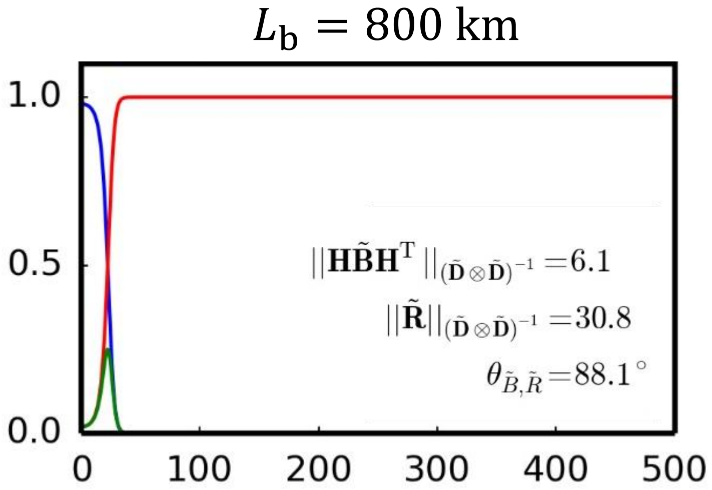
Spectral Distinctiveness of Filters

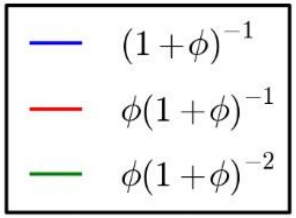
$$\left\|\mathbf{H}\tilde{\mathbf{B}}\mathbf{H}^{\mathrm{T}}\right\|^{2}_{(\tilde{\mathbf{D}}\otimes\tilde{\mathbf{D}})^{-1}} = \mathrm{Tr}[\tilde{\mathbf{F}}\tilde{\mathbf{F}}] = \sum_{i}\frac{1}{(1+\phi_i)^2}$$

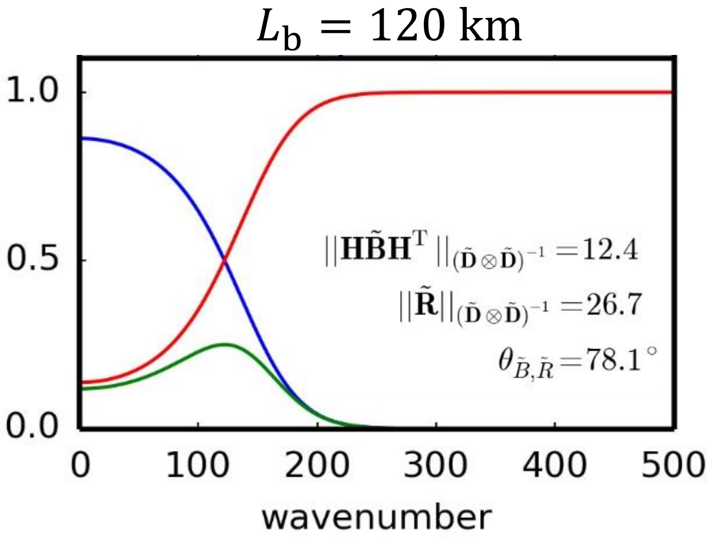
$$\left\|\tilde{\mathbf{R}}\right\|^{2}_{(\tilde{\mathbf{D}}\otimes\tilde{\mathbf{D}})^{-1}} = \mathrm{Tr}[(\mathbf{I}-\tilde{\mathbf{F}})(\mathbf{I}-\tilde{\mathbf{F}})] = \sum_{i}\frac{\phi_i^2}{(1+\phi_i)^2}$$

$$\left\langle\mathbf{H}\tilde{\mathbf{B}}\mathbf{H}^{\mathrm{T}},\tilde{\mathbf{R}}\right\rangle_{(\tilde{\mathbf{D}}\otimes\tilde{\mathbf{D}})^{-1}} = \mathrm{Tr}[\tilde{\mathbf{F}}(\mathbf{I}-\tilde{\mathbf{F}})] = \sum_{i}\frac{\phi_i}{(1+\phi_i)^2}$$

$$\cos\left(\theta_{\tilde{B},\tilde{R}}\right) = \frac{\left\langle\mathbf{H}\tilde{\mathbf{B}}\mathbf{H}^{\mathrm{T}},\tilde{\mathbf{R}}\right\rangle_{(\tilde{\mathbf{D}}\otimes\tilde{\mathbf{D}})^{-1}}}{\left\|\mathbf{H}\tilde{\mathbf{B}}\mathbf{H}^{\mathrm{T}}\right\|_{(\tilde{\mathbf{D}}\otimes\tilde{\mathbf{D}})^{-1}}\times\left\|\tilde{\mathbf{R}}\right\|_{(\tilde{\mathbf{D}}\otimes\tilde{\mathbf{D}})^{-1}}}$$







Limiting Cases

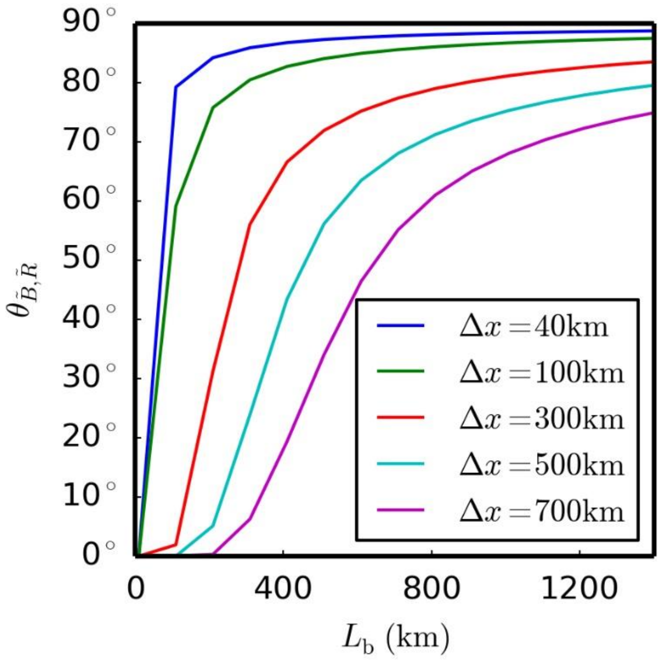
- 1D periodic domain with $L_\mathrm{b} \to \infty$, $L_\mathrm{o} \to 0$:
  - Only one overlapping wavenumber

$$\cos\left(\theta_{\tilde{B},\tilde{R}}\right) = \frac{1}{\sqrt{\left(1+\frac{1}{\phi_0}\right)^2 \left(\frac{L}{\Delta x}-1\right)+1}} \qquad \theta_{\tilde{B},\tilde{R}} \xrightarrow{\Delta x \to 0} 90°$$

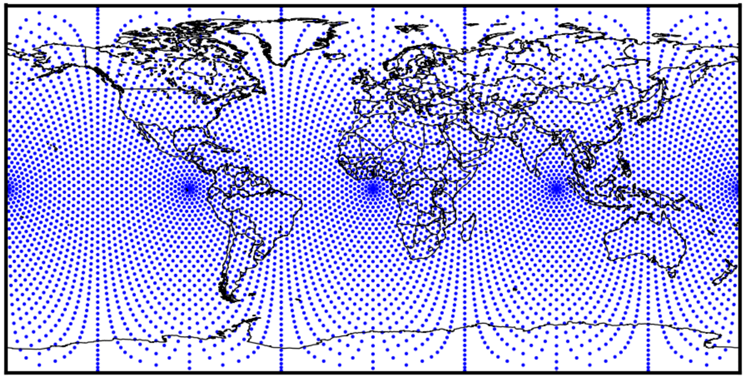
- $\mathbf{H\tilde{B}H}^\mathrm{T} \propto \mathbf{\tilde{R}}$:
  - $\mathbf{\tilde{F}}$ and $\mathbf{I}+\mathbf{\tilde{F}}$ have flat spectra

$$\theta_{\tilde{B},\tilde{R}} = 0°$$

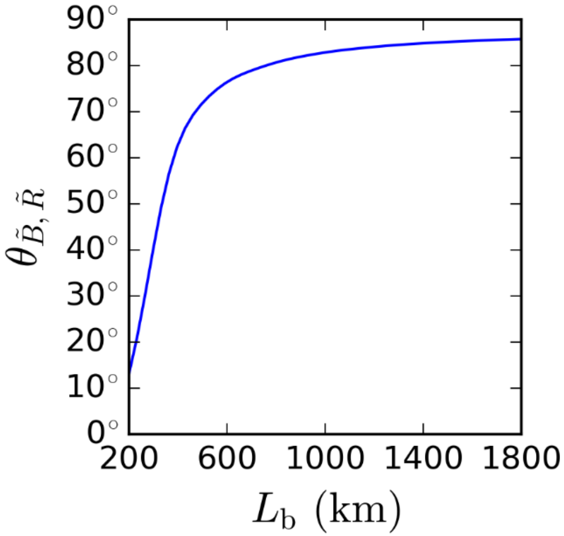
Angles Between Error Covariances



1D periodic domain
$L = 40{,}000$ km, $\tilde{\sigma}_\mathrm{b}^2 = \tilde{\sigma}_\mathrm{o}^2$, $L_\mathrm{o} = 0$

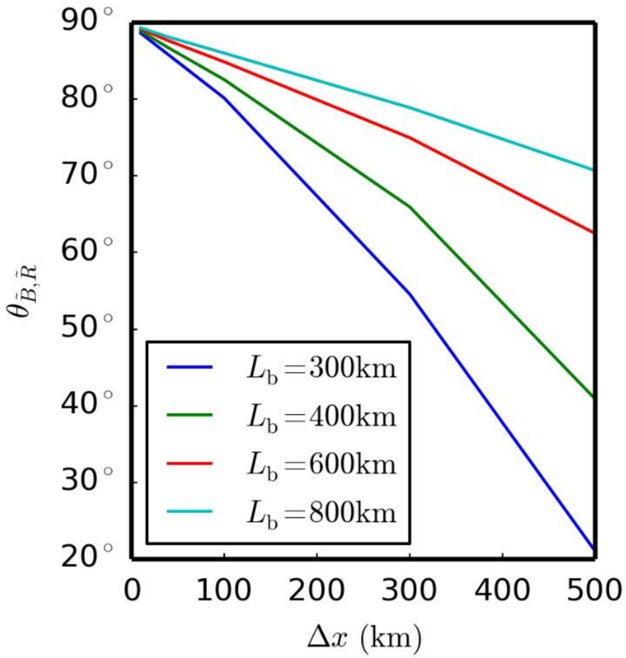


5810-point Lebedev grid, $\Delta x \sim 100$ km $-$ 330 km



$\tilde{\sigma}_\mathrm{b}^2 = \tilde{\sigma}_\mathrm{o}^2$, $L_\mathrm{o} = 0$

Angles Between Error Covariances



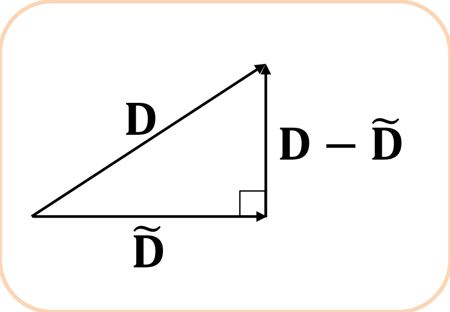
1D periodic domain

$L = 40{,}000$ km, $\tilde{\sigma}_b^2 = \tilde{\sigma}_o^2$, $L_o = 0$

χ^2 Diagnostic

- Weighting of $(\tilde{\mathbf{D}}_B \otimes \tilde{\mathbf{D}}_B)^{-1}$ and $(\tilde{\mathbf{D}}_R \otimes \tilde{\mathbf{D}}_R)^{-1}$gives algorithm to satisfy the χ^2 diagnostic with $\hat{s}_\mathrm{b} = \hat{s}_\mathrm{o}$

$$\chi^2 \text{ diagnostic satisfied if } \left\langle \tilde{\mathbf{D}}, \mathbf{D} \right\rangle_{(\tilde{\mathbf{D}} \otimes \tilde{\mathbf{D}})^{-1}} = \left\| \tilde{\mathbf{D}} \right\|^2_{(\tilde{\mathbf{D}} \otimes \tilde{\mathbf{D}})^{-1}} = N_\mathrm{obs}$$



$$\left\| \mathbf{D} - \tilde{\mathbf{D}} \right\|^2_{(\tilde{\mathbf{D}} \otimes \tilde{\mathbf{D}})^{-1}} = \left\| \mathbf{D} \right\|^2_{(\tilde{\mathbf{D}} \otimes \tilde{\mathbf{D}})^{-1}} - \left\| \tilde{\mathbf{D}} \right\|^2_{(\tilde{\mathbf{D}} \otimes \tilde{\mathbf{D}})^{-1}}$$

Comparing to Hollingsworth and Lönnberg

- First minimize $J_B^{\mathrm{HL}} = \frac{1}{2}\left\| s_\mathrm{b}\mathbf{V}\circ\widetilde{\mathbf{D}} - \mathbf{V}\circ\mathbf{D}\right\|^2_{(\widetilde{\boldsymbol{\Sigma}}_\mathrm{b}^2\otimes\widetilde{\boldsymbol{\Sigma}}_\mathrm{b}^2)^{-1}}$

minimize w.r.t. S_b

$$s_\mathrm{b}^{\mathrm{HL}} = \frac{\left\langle \mathbf{V}\circ\widetilde{\mathbf{D}}, \mathbf{V}\circ\mathbf{D}\right\rangle_{(\widetilde{\boldsymbol{\Sigma}}_\mathrm{b}^2\otimes\widetilde{\boldsymbol{\Sigma}}_\mathrm{b}^2)^{-1}}}{\left\|\mathbf{V}\circ\widetilde{\mathbf{D}}\right\|^2_{(\widetilde{\boldsymbol{\Sigma}}_\mathrm{b}^2\otimes\widetilde{\boldsymbol{\Sigma}}_\mathrm{b}^2)^{-1}}}$$

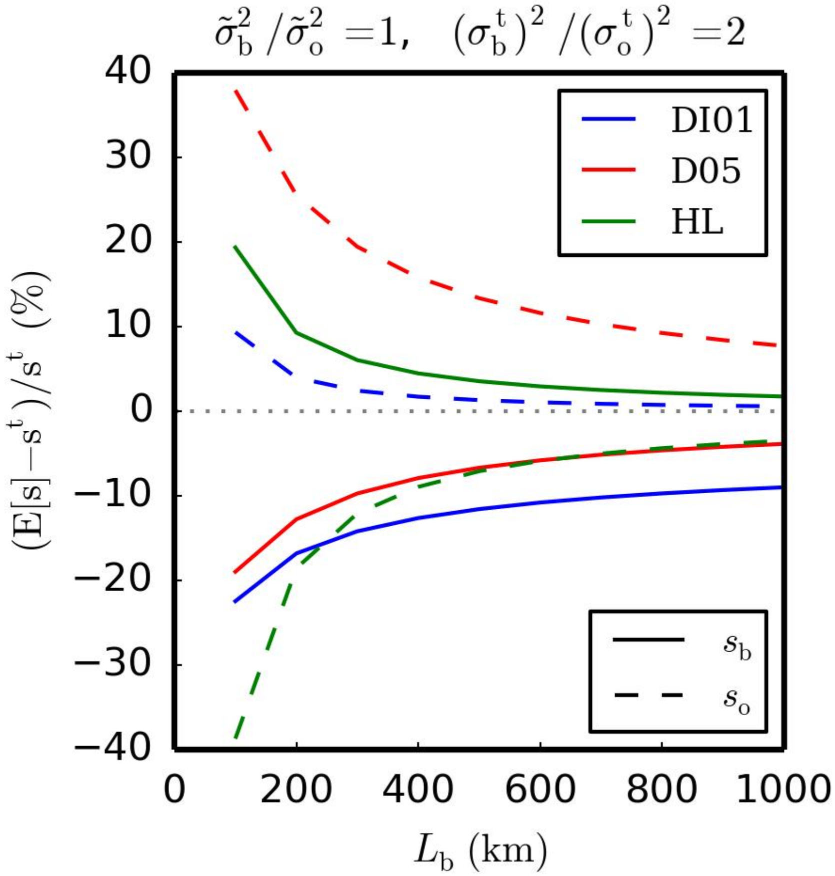
$$\mathbf{V} \equiv \begin{bmatrix} 0 & 1 & 1 & \\ 1 & 0 & 1 & \cdots \\ 1 & 1 & 0 & \\ & \vdots & & \ddots \end{bmatrix}$$

- Then minimize $J_R^{\mathrm{HL}} = \frac{1}{2}\left\| \mathbf{I}\circ\left(s_\mathrm{b}^{\mathrm{HL}}\mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^\mathrm{T} + s_\mathrm{o}\widetilde{\mathbf{R}}\right) - \mathbf{I}\circ\mathbf{D}\right\|^2_{(\widetilde{\boldsymbol{\Sigma}}_\mathrm{o}^2\otimes\widetilde{\boldsymbol{\Sigma}}_\mathrm{o}^2)^{-1}}$

minimize w.r.t. S_o

$$s_\mathrm{o}^{\mathrm{HL}} = \frac{\left\langle \mathbf{I}\circ\widetilde{\mathbf{R}}, \mathbf{I}\circ\left(\mathbf{D} - s_\mathrm{b}^{\mathrm{HL}}\mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^\mathrm{T}\right)\right\rangle_{(\widetilde{\boldsymbol{\Sigma}}_\mathrm{o}^2\otimes\widetilde{\boldsymbol{\Sigma}}_\mathrm{o}^2)^{-1}}}{\left\|\mathbf{I}\circ\widetilde{\mathbf{R}}\right\|^2_{(\widetilde{\boldsymbol{\Sigma}}_\mathrm{o}^2\otimes\widetilde{\boldsymbol{\Sigma}}_\mathrm{o}^2)^{-1}}}$$

Comparisons Between Methods



1D periodic domain
$L = 40{,}000$ km, $\Delta x = 40$ km , $L_o = 40$ km